

Hexachloro-1,3-butadiene
87-68-3 | DTXSID7020683

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 |

Model Results

Predicted value: 220 °C

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 8.21e-01

Nearest Neighbors from the Training Set

Image not found

Hexachloro-1,3-butadiene

Measured: 215

Predicted: 220

Image not found

Hexachlorocyclopentadiene

Measured: 239

Predicted: 240

Image not found

1,4-Bis(bromomethyl)benzene

Measured: 245

Predicted: 244

Image not found

2,5-Dibromotoluene

Measured: 236

Predicted: 233

Image not found

Hexachloroacetone

Measured: 203

Predicted: 206